

A QUASINONLOCAL COUPLING METHOD FOR NONLOCAL AND LOCAL DIFFUSION MODELS

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ABSTRACT. In this paper, we extend the idea of “geometric reconstruction” to couple a nonlocal diffusion model directly with the classical local diffusion in one dimensional space. This new coupling framework removes interfacial inconsistency, ensures the flux balance, and satisfies energy conservation as well as the maximum principle, whereas none of existing coupling methods for nonlocal-to-local coupling satisfies all of these properties. We establish the well-posedness and provide the stability analysis of the coupling method. We investigate the difference to the local limiting problem in terms of the nonlocal interaction range. Furthermore, we propose a first order finite difference numerical discretization and perform several numerical tests to confirm the theoretical findings. In particular, we show that the resulting numerical result is free of artifacts near the boundary of the domain where a classical local boundary condition is used, together with a coupled fully nonlocal model in the interior of the domain.

1. INTRODUCTION

Nonlocal continuum models have found interesting applications in a number of important scientific and engineering problems, for example, the phase transition [2, 17], the nonlocal heat conduction [3], fracture and damage in brittle solids [37]. Meanwhile, they can often be linked to classic local continuum models where the latter are known to hold [4, 7, 8, 10, 14, 16, 18–20, 22, 25, 26, 28, 31, 38].

While nonlocal integral-type formulations in a nonlocal continuum model can often provide a more accurate description of physical system, especially near defects and singularities, the nonlocality also increases the computational cost, compared to classical local models based on partial differential equations (PDEs). As a result, it is imperative to employ multiscale methods which can retain accuracy around defect cores while improving efficiency away from singularities through local continuum descriptions. In addition, the nonlocal models usually bring modeling challenges near the boundary, as volumetric boundary conditions are needed that require additional calibrations with the physical system. Improper boundary conditions may create unintended modeling error [9, 11, 13]. It is thus interesting to explore alternatives that enable the use of usual local boundary conditions.

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Key words and phrases. geometric reconstruction, quasinonlocal coupling, well-posedness, physics-preserving, modeling error estimate.

The research of Q. Du and X. Tian is supported in part by the U.S. NSF grants DMS-1558744, AFOSR grant FA9550-14-1-0073 MURI Center for Material Failure Prediction through peridynamics and the ARO MURI Grant W911NF-15-1-0562. The work of X. Li is supported in part by the Simons Foundation Collaboration Grant with award number 16-0458. The work of J. Lu is supported in part by the National Science Foundation under award DMS-1454939.

In the past ten years, a number of strategies have been proposed to couple together local-to-nonlocal or two nonlocal continuum models with different nonlocality. These coupling methods include (1) Arlequin type domain decomposition (see e.g., [21, 32]); (2) Optimal-control based coupling (see e.g., [5, 6]); (3) Morphing approach (see e.g., [27]); (4) Force-based blending mechanism (see e.g., [33, 34]); and (5) Energy-based blending mechanism (see e.g., [1, 12, 39]); just to name a few. Among these multiscale models, some exhibit spurious interfacial forces (“ghost forces”) under uniform strain, while others forgo the need for energy and develop consistent force-based methods which are non-conservative.

Recently, a new symmetric, consistent and stable coupling strategy for nonlocal diffusion problems was developed in [23] which couples two nonlocal operators with different horizon parameters δ_1 and δ_2 . The crucial step in the formulation is the idea of “geometric reconstruction” [15] from the quasinonlocal atomistic-to-continuum method for crystalline solids (see e.g., [15, 24, 29, 30, 35, 36]). In this paper, we extend the “geometric reconstruction” idea to couple the nonlocal diffusion directly with the classical local diffusion in one dimensional space. This new framework leads a coupled model that enjoys linear consistency and preserves the maximum principle. Furthermore, well-posedness of the coupling problem, stability analysis and error estimates are established in this work to ensure the validity and reliability of the modeling approach and computational results.

Let us first review *nonlocal diffusion* equations associated with a positive number δ that characterizes the finite range of nonlocal interaction. We refer to [7] for more detailed studies on nonlocal diffusion equations. Generically, the spatial interactions in a linear nonlocal diffusion equation are characterized by a linear operator \mathcal{L}_δ acting on a function $u = u(x) : \mathbb{R}^d \rightarrow \mathbb{R}$ such that

$$\mathcal{L}_\delta u(x) = 2 \int_{\mathbb{R}^d} (u(y) - u(x)) \gamma_\delta(x, y) dy, \quad \forall x \in \Omega, \quad (1.1)$$

for some open domain $\Omega \subset \mathbb{R}^d$. The kernel γ_δ is usually nonnegative, symmetric and translational invariant for isotropic systems. Often it is chosen as a radial function with a compact support, i.e., $\gamma_\delta(x, y) = \gamma_\delta(|x - y|)$ and $\text{supp}(\gamma_\delta) \subset B_\delta(\mathbf{0})$, where $B_\delta(\mathbf{0})$ is the d -dimensional ball of radius δ . The constant $\delta > 0$ is often called a horizon parameter that characterizes the range of nonlocality. We note that the operator \mathcal{L}_δ can be written in the form of $\mathcal{L}_\delta = \mathcal{D} \gamma_\delta \mathcal{D}^*$ where \mathcal{D} and \mathcal{D}^* are some basic nonlocal operators defined in a nonlocal vector calculus given in [8]. Such a formulation naturally draws an analogy between the nonlocal operator \mathcal{L}_δ and the local second order elliptic differential operator $\nabla \cdot (\mathbf{C} \nabla)$. Thus the nonlocal diffusion problems can be studied and compared with the classical diffusion problems. The nonlocal equations defined on the domain Ω are complemented by the “Dirichlet type” boundary conditions, which are constraints on a domain with nonzero d -dimensional volume. Thus we arrive at the steady-state nonlocal volume-constrained diffusion problem:

$$\begin{cases} -\mathcal{L}_\delta u = f & \text{on } \Omega, \\ u = 0 & \text{on } \Omega_{\mathcal{I}} \end{cases} \quad (1.2)$$

for a function $u(x) : \mathbb{R}^d \rightarrow \mathbb{R}$ and $\Omega_{\mathcal{I}}$ being the nonlocal interaction domain of nonzero d -dimensional volume.

To make connections of equation (1.2) with their local differential counterparts, we usually consider the kernel γ_δ to be suitably localized as $\delta \rightarrow 0$. Without being too technical, this essentially means that we want $\gamma_\delta(|x|)|x|^2$ to be approximating the Dirac delta measure at the origin as $\delta \rightarrow 0$. Often, a convenient assumption for us to make is that γ_δ is a rescaled kernel,

$$(K) \quad \begin{cases} \gamma_\delta(|x|) = \frac{1}{\delta^{d+2}} \gamma\left(\frac{|x|}{\delta}\right), & \gamma \text{ is nonnegative and nonincreasing on } (0, 1), \\ \text{with } \text{supp}(\gamma) \subset [0, 1] \text{ and } \int_{\mathbb{R}^d} |x|^2 \gamma(|x|) dx = d. \end{cases}$$

In this paper, we propose an energy-based coupling method that combines the nonlocal diffusion equation defined as above with the local classical diffusion equation. Since the construction of our coupling follows the spirit of the quasinonlocal atomistic-to-continuum coupling methods for crystalline materials (see for example, [15, 24, 29, 30, 35, 36]), we call our coupling method the *quasinonlocal (QNL) coupling* of nonlocal and local diffusion. We focus on one-dimensional problems in this work to better illustrate the idea. The multi-dimensional generalizations are possible and will be carried out in separate works.

More specifically, in section 2 we first define the combined total energy from which the quasinonlocal operator is derived through energy variation, followed by the discussion of the concerned issue of patch-test consistency. Section 3 contains rigorous arguments of the well-posedness of the coupled problem. Section 4 further explores the modeling accuracy of the coupled method compared with the fully local diffusion equation in terms of small δ , in which the uniform first order accuracy in terms of δ is shown. Section 5 contains numerical experiments and then conclusion and discussions are put in section 6.

2. CONSISTENT COUPLING OF NONLOCAL AND LOCAL DIFFUSIONS

In this section, we formulate our idea of QNL coupling in a one-dimensional bar. Without loss of generality, we work on the domain $\Omega = (-1, 1)$ throughout the paper. We consider the nonlocal interaction region to be on the left side of the bar Ω and the local interaction region to be on the right side with a transition layer in the middle of width δ . Now that the domain Ω is composed of both nonlocal and local interaction regions, the Dirichlet boundary condition to impose should be considered as a mixture of nonlocal and local boundary conditions. Specifically, to the left of the bar Ω there is a nonlocal boundary $(-1 - \delta, -1)$ and to the right of the bar a local boundary $\{1\}$. In all further discussions we use $\Omega_\delta = (-1 - \delta, -1) \cup \{1\}$ as the boundary domain which is mixed with nonlocal and local boundary. See Figure 1 for the graphical illustration of the coupled nonlocal and local domain.

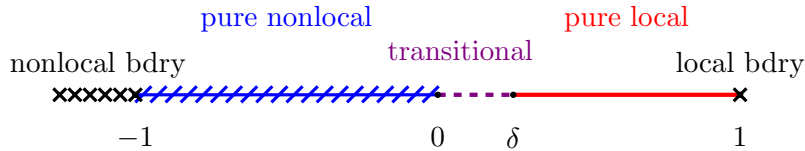


FIGURE 1. Graphical illustration of the 1D domain

2.1. The energy space. The QNL coupling method comes from energy variation of the total energy defined as

$$E_\delta^{\text{qnl}}(u) := \frac{1}{2} \iint_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y - x|) (u(y) - u(x))^2 dy dx + \frac{1}{2} \int_{x > 0} |u'(x)|^2 \omega_\delta(x) dx. \quad (2.1)$$

where the weight function ω_δ is given by

$$\omega_\delta(x) := \int_0^1 dt \int_{|s| < \frac{x}{t}} |s|^2 \gamma_\delta(|s|) ds. \quad (2.2)$$

From the definition of the kernel γ_δ in (K), in particular $\int_{-\delta}^\delta |s|^2 \gamma_\delta(|s|) ds = 1$, it is easy to see that $\omega_\delta(x)$ is a nondecreasing function on $[0, \infty)$ with $\omega_\delta(0) = 0$ and $\omega_\delta(x) = 1$ for $x \geq \delta$. Thus the total quasinonlocal energy has a transition from pure nonlocal to pure local through the transitional region $(0, \delta)$. We further characterize of the weight function $\omega_\delta(x)$ in the following lemma.

Lemma 2.1. *By the definition of ω_δ in (2.2), we have the following equations*

$$\omega_\delta(x) = 2 \int_0^x s^2 \gamma_\delta(|s|) ds + 2x \int_x^\infty s \gamma_\delta(|s|) ds \quad (2.3)$$

$$\omega'_\delta(x) = 2 \int_x^\infty s \gamma_\delta(s) ds \quad (2.4)$$

Proof. For the first equation,

$$\begin{aligned} \omega_\delta(x) &= \int_0^1 dt \int_{|s| < \frac{x}{t}} s^2 \gamma_\delta(|s|) ds = 2 \int_0^1 dt \int_0^{\frac{x}{t}} s^2 \gamma_\delta(|s|) ds \\ &= 2 \int_0^x s^2 \gamma_\delta(|s|) \int_0^1 dt ds + 2 \int_x^\infty s^2 \gamma_\delta(|s|) \int_0^{\frac{x}{s}} dt ds \\ &= 2 \int_0^x s^2 \gamma_\delta(|s|) ds + 2x \int_x^\infty s \gamma_\delta(|s|) ds. \end{aligned}$$

Then $\omega'_\delta(x)$ is obtained by taking derivatives of the expression. \square

Remark 2.1. For given kernel γ , we could calculate ω_δ using the formula (2.3) given in the Lemma 2.1. We give two examples in the following and the plot of the corresponding weight function is shown in Figure 2. These kernels will be used in our numerical example too.

(1) $\gamma_\delta(x) = \frac{3}{2\delta^3} \chi_{(-\delta, \delta)}(x)$, then

$$\omega_\delta(x) = \begin{cases} \frac{3x}{2\delta} - \frac{x^3}{2\delta^3} & x \in (0, \delta) \\ 1 & x \geq \delta \end{cases}$$

(2) $\gamma_\delta(x) = \frac{1}{|x|\delta^2} \chi_{(-\delta, \delta)}(x)$, then

$$\omega_\delta(x) = \begin{cases} \frac{2x}{\delta} - \frac{x^2}{\delta^2} & x \in (0, \delta) \\ 1 & x \geq \delta \end{cases}$$

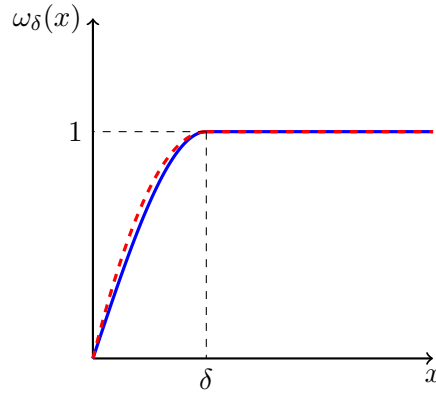


FIGURE 2. Blue line: weight function for $\gamma_\delta(x) = \frac{3}{2\delta^3} \chi_{(-\delta, \delta)}(x)$. Red dashed line: weight function for $\gamma_\delta(x) = \frac{1}{|x|\delta^2} \chi_{(-\delta, \delta)}(x)$.

The energy defined in (2.1) has a more intuitive interpretation from the geometric reconstruction formulation [15, 23, 24]. We will show in Proposition 2.1 that (2.1) is equivalent to the following

$$E_\delta^{\text{qnl}}(u) = \frac{1}{2} \iint_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dy dx \quad (2.5)$$

$$+ \frac{1}{2} \iint_{x > 0 \text{ and } y > 0} dy dx \gamma_\delta(|y-x|) \cdot \int_0^1 dt |u'(x + t(y-x))|^2 |y-x|^2.$$

To better convey the idea of geometric reconstruction proposed in [23], we first assume that $\Omega = \Omega_1 \sqcup \Omega_2$ is dominated by two different nonlocal kernels γ_{δ_1} and γ_{δ_2} ($\delta_2 < \delta_1$), respectively. Next, we utilize the interaction kernel γ_{δ_1} throughout the entire domain Ω , while in the subregion Ω_2 , the displacement of bond $(u(y) - u(x))$ will be *reconstructed* so that it only involves x and y pairs that are closer in distance. More concretely, to link the interaction with kernel γ_{δ_2} to γ_{δ_1} where $\delta_1 = M\delta_2$, if a bond $\{x-y\}$ is completely contained in the subregion Ω_2 , then the displacement of this bond $(u(y) - u(x))$ will be reconstructed by the following expression:

$$u(y) - u(x) \rightarrow \left(u\left(x + \frac{j+1}{M}(y-x)\right) - u\left(x + \frac{j}{M}(y-x)\right) \right) M, \quad \text{for } j = 0, \dots, (M-1).$$

Hence, the bond interaction $\gamma_{\delta_2}(|y-x|) (u(y) - u(x))^2$ in Ω_2 is approximated by

$$\gamma_{\delta_1}(|y-x|) \frac{1}{M} \sum_{j=0}^{M-1} \left(\left(u\left(x + \frac{j+1}{M}(y-x)\right) - u\left(x + \frac{j}{M}(y-x)\right) \right) \frac{\delta_1}{\delta_2} \right)^2. \quad (2.6)$$

Note that if $|x-y| \leq \delta_1$, the difference on the right is evaluated at points with distance at most $\frac{\delta_1}{M} = \delta_2$; thus effectively, the difference $u(y) - u(x)$ is reconstructed by a more local interaction (and hence the idea was referred to as the “geometric reconstruction” scheme in [15]). In fact, if such reconstruction is adopted everywhere in the entire domain Ω , one will recover the fully nonlocal interactions with kernel γ_{δ_2} only [23]. Notice that when $M = \frac{\delta_1}{\delta_2} \rightarrow \infty$, the summation in (2.6) can be viewed as a Riemann sum that converges to an integral, that is

$$\begin{aligned} & \frac{1}{M} \sum_{j=0}^{M-1} \left(\left(u\left(x + \frac{j+1}{M}(y-x)\right) - u\left(x + \frac{j}{M}(y-x)\right) \right) \frac{\delta_1}{\delta_2} \right)^2 \\ &= \sum_{j=0}^{M-1} \left(\frac{u\left(x + \frac{j+1}{M}(y-x)\right) - u\left(x + \frac{j}{M}(y-x)\right)}{\frac{1}{M}(y-x)} (y-x) \right)^2 \frac{1}{M} \\ &\rightarrow \int_0^1 |u'(x + t(y-x))|^2 |y-x|^2 dt \quad \text{as } M \rightarrow \infty. \end{aligned}$$

Therefore, the nonlocal bond interaction $\gamma_\delta(|y-x|) (u(y) - u(x))^2$ can be reconstructed by its local continuum approximation:

$$\gamma_\delta(|y-x|) \cdot \int_0^1 |u'(x + t(y-x))|^2 |y-x|^2 dt. \quad (2.7)$$

Based on this construction, we arrive at the total coupling energy (2.5).

We will show now that the two ways of writing the quasinonlocal total energy are the same. From the expressions (2.1) and (2.5), it suffices to show that local contribution to the total energy is equivalent. The two different ways of writing the local contribution of the energy has their own advantages and we will adopt either definition at our convenience in the sequel.

Proposition 2.1. *The following two expressions of local contribution to the total energy are equivalent*

$$E_\delta^{\text{loc}}(u) = \frac{1}{2} \iint_{x>0 \text{ and } y>0} dx dy \gamma_\delta(|y-x|) \cdot \int_0^1 dt |u'(x+t(y-x))|^2 |y-x|^2, \quad (2.8)$$

and,

$$E_\delta^{\text{loc}}(u) = \frac{1}{2} \int_{x>0} |u'(x)|^2 \omega_\delta(x) dx. \quad (2.9)$$

Proof. We start with recasting the right hand side of (2.8)

$$\begin{aligned} & \frac{1}{2} \iint_{x>0 \text{ and } y>0} \gamma_\delta(|y-x|) \cdot \int_0^1 dt |u'(x+t(y-x))|^2 |y-x|^2 \\ &= \frac{1}{2} \int_0^1 dt \int_{x>0} dx \int_{z>(1-t)x} dz \gamma_\delta\left(\left|\frac{z-x}{t}\right|\right) |u'(z)|^2 \frac{1}{t^3} |z-x|^2 \\ &= \frac{1}{2} \int_0^1 dt \int_{z>0} dz |u'(z)|^2 \int_{0<x<\frac{z}{1-t}} \gamma_\delta\left(\left|\frac{x-z}{t}\right|\right) \frac{1}{t^3} |x-z|^2 dx \\ &= \frac{1}{2} \int_{z>0} dz |u'(z)|^2 \int_0^1 dt \int_{-\frac{z}{t}<s<\frac{z}{1-t}} \gamma_\delta(|s|) |s|^2 ds. \end{aligned}$$

Now since

$$\begin{aligned} & \int_0^1 dt \int_{-\frac{z}{t}<s<\frac{z}{1-t}} |s|^2 \gamma_\delta(|s|) ds \\ &= \int_0^1 dt \int_{-\frac{z}{t}<s<0} |s|^2 \gamma_\delta(|s|) ds + \int_0^1 dt \int_{0<s<\frac{z}{1-t}} |s|^2 \gamma_\delta(|s|) ds \\ &= \int_0^1 dt \int_{-\frac{z}{t}<s<0} |s|^2 \gamma_\delta(|s|) ds + \int_0^1 dt \int_{0<s<\frac{z}{t}} |s|^2 \gamma_\delta(|s|) ds, \end{aligned}$$

we arrive at definition of E_δ^{loc} in (2.9) with the weight function ω_δ as in (2.2). \square

Naturally, we seek solutions in the energy space $\mathcal{S}_\delta^{\text{qnl}}(\Omega)$ equipped with norm

$$\|u\|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}^2 = \|u\|_{L^2(\Omega \cup \Omega_\delta)}^2 + |u|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}^2$$

where $|u|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}^2 := 2E_\delta^{\text{qnl}}(u)$. Now define $\mathcal{S}_\delta^{\text{qnl}}(\Omega)$ to be the completion of $C_c^\infty(\Omega)$ under the norm $\|\cdot\|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}$, namely,

$$\mathcal{S}_\delta^{\text{qnl}}(\Omega) = \{u \in L^2(\Omega \cup \Omega_\delta) : \exists \{u_n\} \in C_c^\infty(\Omega), \|u_n - u\|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)} \rightarrow 0 \text{ as } n \rightarrow \infty\}.$$

Then we know first that $\mathcal{S}_\delta^{\text{qnl}}(\Omega)$ is a Hilbert space with inner product $(\cdot, \cdot)_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}$ to be defined as

$$(u, v)_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)} = (u, v)_{L^2(\Omega \cup \Omega_\delta)} + b_\delta^{\text{qnl}}(u, v)$$

where $b_\delta^{\text{qnl}}(u, v)$ is defined as

$$\begin{aligned} b_\delta^{\text{qnl}}(u, v) &= \iint_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y-x|) (u(y) - u(x)) (v(y) - v(x)) dy dx \\ &\quad + \int_{x>0} u'(x) \cdot v'(x) \omega_\delta(x) dx. \end{aligned} \quad (2.10)$$

Moreover, Poincaré type inequality holds on the space $\mathcal{S}_\delta^{\text{qnl}}(\Omega)$ that is crucial in showing the well-posedness of the variational problem.

Proposition 2.2 (Poincaré inequality). *For $u \in \mathcal{S}_\delta^{\text{qnl}}(\Omega)$, we have the following Poincaré type inequality,*

$$\|u\|_{L^2(\Omega)} \leq C|u|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}, \quad (2.11)$$

where C is independent of u .

Proof. From Proposition 3.1 which will be shown later in section 3, we know that the quasinonlocal energy $|u|_{\mathcal{S}_\delta^{\text{qnl}}(\Omega)}$ is bounded from below by a purely nonlocal energy defined on the entire domain Ω . Thus by the nonlocal Poincaré inequality established previously in many papers, e.g., [7, 28], (2.11) is true. \square

2.2. The QNL operator. We will derive the QNL operator denoted as $\mathcal{L}_\delta^{\text{qnl}}$ from energy variation. We take the first variation of $E_\delta^{\text{qnl}}(u)$ in (2.5) with any test function $v \in C_c^\infty(\Omega)$, and get

$$\begin{aligned} \langle dE_\delta^{\text{qnl}}(u), v \rangle &:= \lim_{\epsilon \rightarrow 0} \frac{E_\delta^{\text{qnl}}(u + \epsilon v) - E_\delta^{\text{qnl}}(u)}{\epsilon} \\ &= \iint_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y - x|) (u(y) - u(x)) (v(y) - v(x)) dy dx + \int_{x > 0} \omega_\delta(x) u'(x) v'(x) dx \\ &= -2 \iint_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y - x|) (u(y) - u(x)) v(x) dy dx - \int_{x > 0} (\omega_\delta(x) u'(x))' v(x) dx, \end{aligned} \quad (2.12)$$

where the last equality comes integration by parts and the fact that $\omega_\delta(0) = 0$. The force formalism $\mathcal{L}_\delta^{\text{qnl}} u(x)$ is negative to the first variation of total energy, and it splits into three cases:

- Case I (nonlocal region): for $x \leq 0$,

$$\mathcal{L}_\delta^{\text{qnl}} u(x) = 2 \int_{y \in \mathbb{R}} \gamma_\delta(|y - x|) (u(y) - u(x)) dy. \quad (2.13)$$

- Case II (transitional region): for $0 < x \leq \delta$,

$$\mathcal{L}_\delta^{\text{qnl}} u(x) = 2 \int_{y < 0} \gamma_\delta(|y - x|) (u(y) - u(x)) dy + (\omega_\delta(x) u'(x))' \quad (2.14)$$

- Case III (local region): for $x > \delta$,

$$\mathcal{L}_\delta^{\text{qnl}} u(x) = (\omega_\delta(x) u'(x))' = u''(x) \quad (2.15)$$

since $\omega_\delta(x) = 1$ for $x \geq \delta$.

Remark 2.2. Since the QNL operator $\mathcal{L}_\delta^{\text{qnl}}$ is defined through the first variation of total energy, $\mathcal{L}_\delta^{\text{qnl}}$ is self-adjoint, that is, from a physical point of view, the force acting on x from y is equal to the force acting on y from x . This symmetry in acting forces guarantees the balance of linear momentum. In addition, this QNL framework ensures the flux balance, and satisfies energy conservation.

2.3. Consistency at the interface. We will show in this part that the QNL coupling is consistent at the interface (in the language of atomistic-to-continuum coupling, it is free of ghost force), namely, for a linear displacement $u^{\text{lin}}(x) = Fx + a$, the force equals zero. For this matter, we only need to worry about the values of $\mathcal{L}_\delta^{\text{qnl}} u^{\text{lin}}$ in the interfacial region, since it is obvious zero in the pure nonlocal and local regions as given by case I and case III in (2.13) and (2.15). For a more general consideration that will also be useful in the next sections, we give the following lemma that involves the operator $\mathcal{L}_\delta^{\text{qnl}}$ acting on smooth functions in the interfacial region. The lemma

states that if δ is small, the QNL diffusion is approximately a local diffusion with effective diffusion constant $a(x)$.

Lemma 2.2. *For any smooth function v ,*

$$\mathcal{L}_\delta^{\text{qnl}} v(x) = a(x)v''(x) + O(\delta\|v'''\|_{C^0}), \quad 0 < x < \delta, \quad (2.16)$$

where a is given by

$$a(x) = 1 - \int_x^\delta s^2 \gamma_\delta(|s|) ds + 2x \int_x^\delta s \gamma_\delta(|s|) ds. \quad (2.17)$$

Proof. For $x \in (0, \delta)$, by the expressions of ω_δ and ω'_δ in Lemma 2.1, we have

$$\begin{aligned} \mathcal{L}_\delta^{\text{qnl}} v(x) &= 2 \int_{y < 0} \gamma_\delta(|y - x|) (v(y) - v(x)) dy + (\omega_\delta(x)v'(x))' \\ &= 2 \int_{-\delta}^{-x} \gamma_\delta(s) \left(sv'(x) + \frac{1}{2}s^2 v''(x) + O(|s|^3 \|v'''\|_{C^0}) \right) + \omega_\delta(x)v''(x) + \omega'_\delta(x)v'(x) \\ &= \left(\int_x^\delta s^2 \gamma_\delta(|s|) ds \right) v''(x) + \omega_\delta(x)v''(x) + O(\delta\|v'''\|_{C^0}) \\ &= \left(1 - \int_x^\delta s^2 \gamma_\delta(|s|) ds + 2x \int_x^\delta s \gamma_\delta(|s|) ds \right) v''(x) + O(\delta\|v'''\|_{C^0}). \end{aligned}$$

□

Remark 2.3. We can further quantify $a(x)$ as follows.

(1) One can show that $\frac{1}{2} \leq a(x) \leq \frac{3}{2}$ for $x \in (0, \delta)$ and $a(\delta) = 1$. Indeed,

$$a(x) \geq 1 - \int_x^\delta s^2 \gamma_\delta(|s|) ds \geq 1 - \int_0^\delta s^2 \gamma_\delta(|s|) ds = \frac{1}{2},$$

and

$$a(x) \leq 1 - \int_x^\delta s^2 \gamma_\delta(|s|) ds + 2 \int_x^\delta s^2 \gamma_\delta(|s|) ds \leq 1 + \int_0^\delta s^2 \gamma_\delta(|s|) ds = \frac{3}{2}.$$

As last, $a(\delta) = 1$ is obvious.

(2) For the two examples that $\gamma_\delta(x) = \frac{3}{2\delta^3} \chi_{(-\delta, \delta)}(x)$ and $\gamma_\delta(x) = \frac{1}{|x|\delta^2} \chi_{(-\delta, \delta)}(x)$, we could calculate $a(x)$ explicitly through equation (2.17).

$$a(x) = \begin{cases} \frac{1}{2} + \frac{3x}{2\delta} - \frac{x^3}{\delta^3} & \text{for } \gamma_\delta(x) = \frac{3}{2\delta^3} \chi_{(-\delta, \delta)}(x) \\ \frac{1}{2} + \frac{2x}{\delta} - \frac{3x^2}{2\delta^2} & \text{for } \gamma_\delta(x) = \frac{1}{|x|\delta^2} \chi_{(-\delta, \delta)}(x). \end{cases}$$

We remark that although the effective local diffusion coefficient $a(x)$ is not equal to a constant one for $0 < x < \delta$, we have in the two cases

$$\int_0^\delta a(x) dx = \delta.$$

In other words, the spacial averaged diffusion coefficient for $0 < x < \delta$ is equal to one.

Lemma 2.2 shows the expansion of $\mathcal{L}_\delta^{\text{qnl}} v(x)$ in the interfacial region using with the second and higher derivatives of v . Thus it is obvious that for a linear function u^{lin} , $\mathcal{L}_\delta^{\text{qnl}} u^{\text{lin}} = 0$. In other words, the QNL coupling passes the patch-test.

Corollary 2.1 (Patch-test consistency). *For a linear function $u^{\text{lin}}(x) = Fx + a$,*

$$\mathcal{L}_\delta^{\text{qnl}} u^{\text{lin}} = 0.$$

Proof. This immediately follows from (2.13), (2.14), and (2.15) using Lemma 2.2. \square

3. STABILITY AND WELL-POSEDNESS

In this section, our goal is to show that the bilinear form $b_\delta^{\text{qnl}}(\cdot, \cdot) : \mathcal{S}_\delta^{\text{qnl}}(\Omega) \times \mathcal{S}_\delta^{\text{qnl}}(\Omega) \rightarrow \mathbb{R}$ defined by (3.4) is bounded and coercive, thus the well-posedness of the variational problem can be followed. The boundedness of the bilinear norm is obvious since $\mathcal{S}_\delta^{\text{qnl}}(\Omega)$ is a Hilbert space and $b_\delta^{\text{qnl}}(\cdot, \cdot)$ is part of its inner product. The coercivity is from the Poincaré inequality (2.11), and the essential step is proved in Proposition 3.1. Now let us define the local contribution of the bilinear form as

$$b_\delta^{\text{loc}}(u, v) := \int_{x>0} u'(x) \cdot v'(x) \omega_\delta(x) dx. \quad (3.1)$$

We can see the lower bound of $b_\delta^{\text{loc}}(u, u)$ in the following lemma.

Lemma 3.1. *For $b_\delta^{\text{loc}}(u, v)$ defined in (3.1), we have*

$$b_\delta^{\text{loc}}(u, u) \geq \iint_{x>0 \text{ and } y>0} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dx dy. \quad (3.2)$$

Proof. The right hand side of (3.2) can be recast as

$$\begin{aligned} & \int_{x>0 \text{ and } y>0} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dx dy \\ &= \int_{x>0} dx \int_{y>0} dy \gamma_\delta(|y-x|) \left[\int_{0<t<1} du(x+t(y-x)) \right]^2 \\ &= \int_{x>0} dx \int_{y>0} dy \gamma_\delta(|y-x|) \left[\int_0^1 (y-x) \cdot u'(x+t(y-x)) dt \right]^2 \\ &\leq \int_{x>0} dx \int_{y>0} dy \gamma_\delta(|y-x|) (y-x)^2 \int_0^1 |u'(x+t(y-x))|^2 dt, \end{aligned} \quad (3.3)$$

where the last expression is exactly $2E_\delta^{\text{loc}}(u) = b_\delta^{\text{loc}}(u, u)$ as shown in Proposition 2.1. \square

Lemma 3.1 immediately leads to the stability property compared to the fully nonlocal bilinear operator.

Proposition 3.1. *For $b_\delta^{\text{qnl}}(u, v)$ defined in (3.1), we have*

$$b_\delta^{\text{qnl}}(u, u) \geq \iint_{x, y \in \mathbb{R}} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dy dx. \quad (3.4)$$

Proof. Recall the definition of $b_\delta^{\text{qnl}}(u, u)$ and use the conclusion of Lemma 3.1, we immediately get

$$\begin{aligned} b_\delta^{\text{qnl}}(u, u) &= \int_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dx dy + b_\delta^{\text{loc}}(u, u) \\ &\geq \int_{x \leq 0 \text{ or } y \leq 0} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dx dy \\ &\quad + \int_{x>0 \text{ and } y>0} \gamma_\delta(|y-x|) (u(y) - u(x))^2 dx dy \end{aligned}$$

\square

Now from the Poincaré inequality Proposition 2.2, we conclude that $b_\delta^{\text{qnl}}(\cdot, \cdot)$ is bounded and coercive, thus leading to the well-posedness of the QNL model.

Theorem 3.1. *The QNL diffusion equation given by*

$$\begin{cases} -\mathcal{L}_\delta^{\text{qnl}} u_\delta^{\text{qnl}}(x) = f(x), & \text{for } x \in \Omega \\ u_\delta(x) = 0, & \text{for } x \in \Omega_\delta \end{cases} \quad (3.5)$$

is well-posed, where $\mathcal{L}_\delta^{\text{qnl}}$ is defined in subsection 2.2.

Proof. The well-posedness follows immediately from Lax-Milgram theorem. \square

4. CONVERGENCE TO THE LOCAL DIFFUSION AS $\delta \rightarrow 0$

We consider in this section the modeling error estimate of the QNL coupling equation (3.5) as $\delta \rightarrow 0$ to the local differential equation

$$\begin{cases} -u_0''(x) = f(x), & x \in \Omega \\ u_0(-1) = u_0(1) = 0. \end{cases} \quad (4.1)$$

In this section we assume that u_0 has a smooth zero extension into $(-1-\delta, -1)$ to avoid discussions on the effect of nonlocal boundary condition there. We denote the error between the solutions to (3.5) and (4.1) to be $e_\delta(x) = u_\delta^{\text{qnl}} - u_0(x)$. With this extension and both local and nonlocal homogeneous Dirichlet conditions imposed on u_δ^{qnl} on the interval $(-1-\delta, -1)$ and the right end point 1 of Ω respectively, we see that $e_\delta(x) = 0$ for $x \in \Omega_\delta$.

Truncation error. Let the truncation error be $T_\delta(x) = \mathcal{L}_\delta^{\text{qnl}} u_0(x) - u_0''(x)$. Then $T_\delta(x) = T_\delta^1(x) + T_\delta^2(x)$, where $T_\delta^1(x) = T_\delta(x)\chi_{(-1,0)}(x)$ and $T_\delta^2(x) = T_\delta(x)\chi_{(0,\delta)}(x)$. According to the calculations in section 2.3, we know that $T_\delta^1(x) = O(\delta^2)$ for $x \in (-1, 0)$ and $T_\delta^2(x) = O(1)$ for $x \in (0, \delta)$. Notice that from Lemma 2.2, for $x \in (0, \delta)$,

$$\begin{aligned} T_\delta^2(x) &= \mathcal{L}_\delta^{\text{qnl}} u_0(x) - u_0''(x) = a(x)u_0''(x) - u_0''(x) + O(\delta) \\ &= \left(2x \int_x^\delta s\gamma_\delta(s)ds - \int_x^\delta s^2\gamma_\delta(s)ds\right)u_0''(x) + O(\delta). \end{aligned}$$

So

$$|T_\delta^2(x)| \leq 3C^* \int_x^\delta s^2\gamma_\delta(s)ds + O(\delta),$$

where $C^* = \|u_0\|_{C^2}$. Now that $-\mathcal{L}_\delta^{\text{qnl}} e_\delta(x) = -\mathcal{L}_\delta^{\text{qnl}} u_\delta^{\text{qnl}}(x) + \mathcal{L}_\delta^{\text{qnl}} u_0(x) = T_\delta(x)$, we have $e_\delta(x) = (-\mathcal{L}_\delta^{\text{qnl}})^{-1}T_\delta^1(x) + (-\mathcal{L}_\delta^{\text{qnl}})^{-1}T_\delta^2(x) = e_\delta^1(x) + e_\delta^2(x)$, where $e_\delta^1(x)$ and $e_\delta^2(x)$ are defined as

$$\begin{cases} e_\delta^1(x) = (-\mathcal{L}_\delta^{\text{qnl}})^{-1}T_\delta^1(x), \\ e_\delta^2(x) = (-\mathcal{L}_\delta^{\text{qnl}})^{-1}T_\delta^2(x). \end{cases} \quad (4.2)$$

We are going to show next that $|e_\delta^1(x)| = O(\delta^2)$ and $|e_\delta^2(x)| = O(\delta)$. Thus the total error is of order $O(\delta)$. The main ingredients are maximum principle and barrier functions.

In the following, we will show a maximum principle for solutions of (3.5) that may have discontinuity at 0. We need such result for error estimate because the truncation error T_δ has been decomposed into two piecewise smooth functions such that e_δ^1 and e_δ^2 might be discontinuous at 0.

Lemma 4.1 (Maximum principle). *The operator $\mathcal{L}_\delta^{\text{qnl}}$ satisfies the maximum principle, namely, if $u \in C([-1, 0]) \cap C^2([0, 1])$, then $-\mathcal{L}_\delta^{\text{qnl}} u(x) \leq 0$ in Ω implies that,*

$$\max_{x \in \Omega \cup \Omega_\delta} u(x) \leq \max_{x \in \Omega_\delta} u(x).$$

Proof. First, from $-\mathcal{L}_\delta^{\text{qnl}}u(x) \leq 0$ in $(0, 1)$ we can show that

$$\max_{x \in (0, 1)} u(x) \leq \max_{x \in \{0^+\} \cup \{1\}} u(x), \quad (4.3)$$

where $u(0^+) = \lim_{x \rightarrow 0, x > 0} u(x)$. Indeed, if we assume the opposite is true, namely if $\tilde{x} \in (0, 1)$ is an isolated maximum point, then we must have $u'(\tilde{x}) = 0$ and $u'(\tilde{x}) < 0$. From the expressions of $\mathcal{L}_\delta^{\text{qnl}}$ in (2.14) and (2.15), we have immediately $-\mathcal{L}_\delta^{\text{qnl}}u(\tilde{x}) > 0$, which contradicts the assumption. Second, from $-\mathcal{L}_\delta^{\text{qnl}}u(x) \leq 0$ in $[-1, 0]$ we could show

$$\max_{x \in (-1-\delta, \delta)} u(x) \leq \max_{x \in (-1-\delta, -1) \cup (0, \delta)} u(x). \quad (4.4)$$

The argument is the following. Assume the opposition is true, namely,

$$\max_{x \in (-1-\delta, \delta)} u(x) > \max_{x \in (-1-\delta, -1) \cup (0, \delta)} u(x),$$

then we could find $x^* \in [-1, 0]$ such that $u(x^*) = \max_{x \in (-1, 0)} u(x)$ and

$$-\mathcal{L}_\delta^{\text{qnl}}u(x^*) = - \int_{-\delta}^{\delta} \gamma_\delta(|s|)(u(x^* + s) - u(x^*))ds > 0,$$

which gives us a contradiction. So u has to satisfy (4.4).

Now combine the result of (4.3) and (4.4), we only need to show $u(0^+) \leq \max_{x \in \Omega_\delta} u(x)$. Assume the opposite, namely $u(0^+) > u(x)$ for any $x \in [-1 - \delta, 0^-] \cup (0, 1]$. Then since $u(0^+) > u(0^-)$, we have $\int_{y < 0} \gamma_\delta(|y - x|)(u(y) - u(x))dy < 0$ for sufficiently small $x > 0$. Considering also that $u'(0^+) \leq 0$ (since $u(0^+) > u(x)$ for any $x > 0$) and $\omega_\delta(0^+) = 0$, we see that for small enough $x > 0$,

$$-\mathcal{L}_\delta^{\text{qnl}}u(x) = -2 \int_{y < 0} \gamma_\delta(|y - x|)(u(y) - u(x))dy - \omega_\delta(x)u''(x) - \omega'_\delta(x)u'(x) > 0,$$

which gives us a contradiction. □

Theorem 4.1. Suppose u_δ^{qnl} and u_0 are strong solutions to (3.5) and (4.1) respectively. Assume that $u_0 \in C^3(\overline{\Omega \cup \Omega_\delta})$, then

$$\|u_\delta^{\text{qnl}}(x) - u_0(x)\|_{L^\infty(\Omega)} = O(\delta).$$

Proof. We will construct barrier functions and then estimate $e_\delta^1(x)$ and $e_\delta^2(x)$ defined by (4.2). The first barrier function is a simple quadratic function. Take $\Phi_1(x) = -cx^2 + 4c$, then from the calculations in section 2.3 we know that $-\mathcal{L}_\delta^{\text{qnl}}(\delta\Phi_1(x)) \geq c\delta$. For $u_0 \in C^3(\overline{\Omega \cup \Omega_\delta})$, we know that $T_\delta^1(x)$ is at least of order $O(\delta)$, so by choosing c large enough we could have $c\delta \geq T_\delta^1(x)$. Now from Lemma 4.1 we conclude that

$$\max_{x \in \Omega \cup \Omega_\delta} (e_\delta^1(x) - \delta\Phi_1(x)) \leq \max_{x \in \Omega_\delta} (e_\delta^1(x) - \delta\Phi_1(x)) \leq 0,$$

so we have $e_\delta^1(x) \leq \delta\Phi_1(x) \leq 4c\delta$. Applying the same arguments to $-e_\delta^1(x)$ we also have $-e_\delta^1(x) \leq 4c\delta$. Thus $|e_\delta^1(x)| = O(\delta)$.

The second barrier function $\Phi_2(x)$ is more carefully designed in order to get the estimate of $e_\delta^2(x)$. The key is to define $\Phi_2(x)$ in a way that it is C^2 and linear outside the interfacial region $(0, \delta)$. We define the barrier function $\Phi_2(x)$ to be

$$\Phi_2(x) = \begin{cases} \delta x + \delta + \delta^2 & x \in (-1 - \delta, -\delta) \\ \frac{1}{8\delta^2}x^4 - \frac{3}{4}x^2 + \delta + \frac{5}{8}\delta^2 & x \in [-\delta, \delta] \\ -\delta x + \delta + \delta^2 & x \in [\delta, 1]. \end{cases} \quad (4.5)$$

One could check that $\Phi_2 \in C^2(\Omega) \cup C(\overline{\Omega \cup \Omega_\delta})$ and $-\mathcal{L}_\delta^{\text{qnl}}(\Phi_2(x)) \geq 0$ for $x \in (-1, 1)$. In particular, for $x \in (0, \delta)$, after taking Taylor-expansion, we can write

$$\begin{aligned}
-\mathcal{L}_\delta^{\text{qnl}}(\Phi_2(x)) &= -a(x)\Phi_2''(x) - 2 \int_{-\delta}^{-x} \gamma_\delta(s) \left(\frac{1}{6}s^3\Phi_2'''(x) + \frac{1}{24}s^4\Phi_2''''(x) + O(|s|^5)ds \right) \\
&= - \left(1 - \int_x^\delta s^2\gamma_\delta(s)ds + 2x \int_x^\delta s\gamma_\delta(s)ds \right) \Phi_2''(x) \\
&\quad - \frac{1}{3} \left(\int_{-\delta}^{-x} s^3\gamma_\delta(s)ds \right) \Phi_2'''(x) - \frac{1}{12} \left(\int_{-\delta}^{-x} s^4\gamma_\delta(s)ds \right) \Phi_2''''(x) \\
&\geq - \left(\int_{-\delta}^x s^2\gamma_\delta(s)ds + 2 \int_x^\delta s^2\gamma_\delta(s)ds \right) \left(\frac{3}{2} \frac{x^2}{\delta^2} - \frac{3}{2} \right) \\
&\quad + \frac{x}{3} \left(\int_x^\delta s^2\gamma_\delta(s)ds \right) \frac{3x}{\delta^2} - \frac{\delta^2}{12} \left(\int_x^\delta s^2\gamma_\delta(s)ds \right) \frac{3}{\delta^2} \\
&\geq \int_x^\delta s^2\gamma_\delta(s)ds \left(\frac{11}{4} - 2 \frac{x^2}{\delta^2} \right) \geq \frac{3}{4} \int_x^\delta s^2\gamma_\delta(s)ds.
\end{aligned}$$

Then we could take a $\tilde{c} > 0$ large enough such that $-\mathcal{L}_\delta^{\text{qnl}}(\tilde{c}\Phi_2(x)) \geq T_\delta^2(x)$, then from the maximum principle we conclude that

$$\max_{x \in \Omega \cup \Omega_\delta} (e_\delta^2(x) - \tilde{c}\Phi_2(x)) \leq \max_{x \in \Omega_\delta} (e_\delta^2(x) - \tilde{c}\Phi_2(x)) \leq 0.$$

So we have $e_\delta^2(x) \leq \tilde{c}\Phi_2(x) \leq \tilde{c}(\delta + \frac{5}{8}\delta^2)$. Using the same arguments to $-e_\delta^2(x)$ we also have $-e_\delta^2(x) \leq \tilde{c}(\delta + \frac{5}{8}\delta^2)$. Thus $|e_\delta^2(x)| = O(\delta)$. \square

5. NUMERICAL DISCRETIZATION AND NUMERICAL EXAMPLES

In this section, we will develop a finite difference discretization and consider several benchmark problems to check the accuracy and stability performance of the numerical scheme. The patch-test consistency, symmetry and positive definiteness of the finite difference matrix are validated numerically.

5.1. Numerical scheme. We use finite difference for spatial discretization. The domain $\Omega = (-1, 1)$ is divided into $2N$ uniform subintervals with equal length $h = 1/N$ and grid points $-1 = x_0 < x_1 < \dots < x_{2N} = 1$ so the interface grid point is $x_N = 0$. Homogeneous Dirichlet boundary condition $u = 0$ is assumed on the boundary domain $\Omega_\delta = (-\delta - 1, -1) \cup \{1\}$. We use the scaling invariance of second moments of γ_δ and local diffusion and approximate the quasinonlocal diffusion operator $\mathcal{L}_\delta^{\text{qnl}}$ in the three regimes. The finite difference scheme we uses is not only a convergent scheme for the QNL problem with fixed δ , but also a convergent scheme for the local differential equation with fixed ratio between δ and h , thus an asymptotically compatible scheme, a notion developed in [40, 41].

For simplicity of discussion, we always assume that $\delta/h = r$ with r being an integer in the following. We discuss in order the discretization scheme in the nonlocal region, transitional region and local region respectively. Special treatment is used in the transitional region for the scheme to be asymptotically compatible.

- Case I (nonlocal region): for $i \in \{0, 1, \dots, N\}$,

$$\begin{aligned}\mathcal{L}_\delta^{\text{qnl}} u(x_i) &= 2 \int_{-\delta}^{\delta} (u(x_i + s) - u(x_i)) \gamma_\delta(s) ds \\ &= 2 \int_0^\delta \left(\frac{u(x_i + s) - 2u(x_i) + u(x_i - s)}{s^2} \right) s^2 \gamma_\delta(s) ds \\ &\approx 2 \sum_{j=1}^r \left(\frac{u(x_{i+j}) - 2u(x_i) + u(x_{i-j}))}{(jh)^2} \right) \int_{(j-1)h}^{jh} s^2 \gamma_\delta(s) ds.\end{aligned}\tag{5.1}$$

- Case II (transitional region): for $i \in \{N + 1, N + 2, \dots, N + r\}$

$$\begin{aligned}\mathcal{L}_\delta^{\text{qnl}} u(x_i) &= 2 \int_{x_i}^{\delta} \gamma_\delta(|s|) (u(x_i - s) - u(x_i)) ds + 2 \left(\int_{x_i}^{\delta} s \gamma_\delta(s) ds \right) u'(x_i) \\ &\quad + \left(2 \int_0^{x_i} s^2 \gamma_\delta(|s|) ds + 2x_i \int_{x_i}^{\delta} s \gamma_\delta(|s|) ds \right) u''(x_i).\end{aligned}\tag{5.2}$$

Now we split the nonlocal integral term into diffusion part and convection part:

$$\begin{aligned}& 2 \int_{x_i}^{\delta} \gamma_\delta(|s|) (u(x_i - s) - u(x_i)) ds \\ &= \int_{x_i}^{\delta} \gamma_\delta(|s|) (u(x_i + s) - 2u(x_i) + u(x_i - s)) ds - \int_{x_i}^{\delta} \gamma_\delta (u(x_i + s) - u(x_i - s)) ds.\end{aligned}$$

From here we derive the discretization for $\mathcal{L}_\delta^{\text{qnl}} u(x_i)$:

$$\begin{aligned}\mathcal{L}_\delta^{\text{qnl}} u(x_i) &\approx \sum_{j=x_i/h}^r \frac{u(x_{i+j}) - 2u(x_i) + u(x_{i-j}))}{(jh)^2} \int_{(j-1)h}^{jh} s^2 \gamma_\delta(s) ds \\ &\quad - \sum_{j=x_i/h}^r \frac{u(x_{i+j}) - u(x_{i-j}))}{jh} \int_{(j-1)h}^{jh} s \gamma_\delta(s) ds + 2 \left(\int_{x_i}^{\delta} s \gamma_\delta(s) ds \right) \frac{u(x_{i+1}) - u(x_i)}{h} \\ &\quad + \left(2 \int_0^{x_i} s^2 \gamma_\delta(|s|) ds + 2x_i \int_{x_i}^{\delta} s \gamma_\delta(|s|) ds \right) \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1}))}{h^2}.\end{aligned}\tag{5.3}$$

- Case III (local region): for $i \in \{N + r + 1, \dots, 2N\}$,

$$\mathcal{L}_\delta^{\text{qnl}} u(x_i) = u''(x_i) \approx \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1}))}{h^2}.\tag{5.4}$$

Remark 5.1. The finite difference discretization described above is a first order scheme with respect to h for fixed horizon δ to the QNL equation (3.5), as well as a first order scheme for fixed ratio r between δ and h to the local equation (4.1). We split the convection and diffusion parts in (5.2) to balance the convection from nonlocal and local contributions. The resulting discretized expression (5.3) will be asymptotically compatible to the local equation. Otherwise, direct discretization of (5.2) will lead to artificial convection terms and thus it will cause numerical inconsistency and instability on the interfacial regions.

Remark 5.2. For the general case that the interface is at $x^* \neq 0$, we have the following formulas in replace of equation (5.2). If x^* is at the left side of the transitional region, then (5.2) is replace by

$$\begin{aligned}\mathcal{L}_\delta^{\text{qnl}} u(x_i) &= 2 \int_{x_i - x^*}^{\delta} \gamma_\delta(|s|) (u(x_i - s) - u(x_i)) ds + 2 \left(\int_{x_i - x^*}^{\delta} s \gamma_\delta(s) ds \right) u'(x_i) \\ &\quad + \left(2 \int_0^{x_i - x^*} s^2 \gamma_\delta(|s|) ds + 2(x_i - x^*) \int_{x_i - x^*}^{\delta} s \gamma_\delta(|s|) ds \right) u''(x_i).\end{aligned}$$

If x^* is at the right side of the transitional region, then (5.2) is replaced by

$$\begin{aligned} \mathcal{L}_\delta^{\text{qnl}} u(x_i) = & 2 \int_{x^*-x_i}^\delta \gamma_\delta(|s|) (u(x_i + s) - u(x_i)) ds - 2 \left(\int_{x^*-x_i}^\delta s \gamma_\delta(s) ds \right) u'(x_i) \\ & + \left(2 \int_0^{x^*-x_i} s^2 \gamma_\delta(|s|) ds + 2(x^* - x_i) \int_{x^*-x_i}^\delta s \gamma_\delta(|s|) ds \right) u''(x_i). \end{aligned}$$

5.2. Numerical experiments. We solve the QNL problem (3.5) with right hand side f to be

$$f(x) = -12x^2 + 4.$$

The exact solution for the limiting local diffusion problem (4.1) is

$$u_0 = (1 - x)^2(1 + x)^2 \quad \text{for } x \in \Omega. \quad (5.5)$$

We adopt the discretization scheme described in section 5.1 and compute the QNL solution with the ratio between δ and spatial step size h to be fixed. Two types of kernels are used with one being $\gamma_\delta(x) = \frac{3}{2\delta^3} \chi_{(-\delta, \delta)}(x)$ and another being $\gamma_\delta(x) = \frac{1}{\delta^2|x|} \chi_{(-\delta, \delta)}(x)$. We compute first the L^∞ difference between the QNL solution and the local solution and then the L^∞ difference of the gradients which are approximated by second order central finite difference at the mesh points. First order convergences with respect to h are observed in both cases. The results are listed in Table 1 and 2.

h	$\ u_\delta^{\text{qnl}} - u_0\ _{L^\infty}$	Order	$\ (u_\delta^{\text{qnl}} - u_0)'\ _{L^\infty}$	Order
1/50	1.56e-2	—	1.91e-2	—
1/100	8.07e-3	0.95	9.61e-3	0.99
1/200	4.10e-3	0.98	4.82e-3	0.99
1/400	2.06e-3	0.99	2.42e-3	1.00
1/800	1.04e-3	0.99	1.21e-3	1.00

TABLE 1. L^∞ differences of solutions u_δ^{qnl} to u_0 and their gradients. We fix $\delta = 3h$ and the kernel function is $\gamma_\delta(x) = \frac{3}{2\delta^3} \chi_{(-\delta, \delta)}(x)$.

h	$\ u_\delta^{\text{qnl}} - u_0\ _{L^\infty}$	Order	$\ (u_\delta^{\text{qnl}} - u_0)'\ _{L^\infty}$	Order
1/50	1.19e-2	—	1.80e-2	—
1/100	6.19e-3	0.95	9.13e-3	0.98
1/200	3.14e-3	0.97	4.59e-3	0.99
1/400	1.59e-3	0.99	2.30e-3	1.00
1/800	7.97e-4	0.99	1.15e-3	1.00

TABLE 2. L^∞ differences of solutions u_δ^{qnl} to u_0 and their gradients. We fix $\delta = 3h$ and the kernel function is $\gamma_\delta(x) = \frac{1}{\delta^2|x|} \chi_{(-\delta, \delta)}(x)$.

5.3. Local-nonlocal-local coupling. Volumetric constraints for nonlocal models often cause non-physical boundary layer issues, as shown in Figure 3 (a). We could fix the boundary layer problem by coupling the nonlocal models with local models and remove the volume constraints completely. Figure 3 (b) shows the solution of the local-nonlocal-local coupling with interfaces at $x^a = \frac{-1}{2}$ and $x^b = \frac{1}{2}$. We see that the coupling method removes the artificial boundary layer caused by volume constraints with classical local Dirichlet boundary conditions imposed.

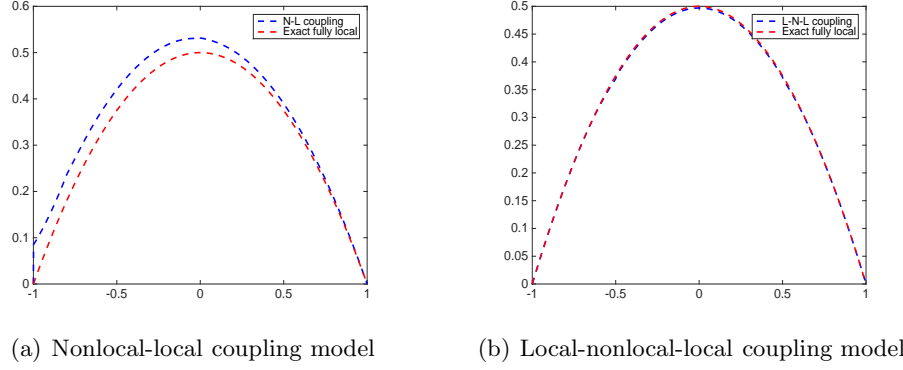


FIGURE 3. Plots of solutions to nonlocal-local coupling model, local-nonlocal-local coupling model and fully local local model with homogeneous Dirichlet boundary condition and right hand side $f \equiv 1$. Kernel function is chosen to be $\gamma_\delta(x) = \frac{3}{2\delta^3}\chi_{(-\delta,\delta)}(x)$. The nonlocal-local coupling model has interface at $x = 0$. The local-nonlocal-local coupling model has interfaces at $x^a = -\frac{1}{2}$ and $x^b = \frac{1}{2}$. The mesh size is $h = 1/800$, the horizon size of nonlocal interaction is $\delta = 0.2$. The nonlocal-local coupling model displays non-physical boundary layer at the nonlocal side, whereas the result of local-nonlocal-local removes the boundary layer.

Next we consider the following singular external forces:

$$f(x) = \frac{(1-x^2)(1+x^2)}{|x-x^*|}, \quad x^* = h/2. \quad (5.6)$$

The solutions for fully nonlocal, local-nonlocal-local coupling and classical local models are plotted in Figure 4. We can see that the local-nonlocal-local coupling not only captures the singular behavior of the nonlocal solution at x^* , but also matches with the local solution at two sides of the bar $(-1, 1)$.

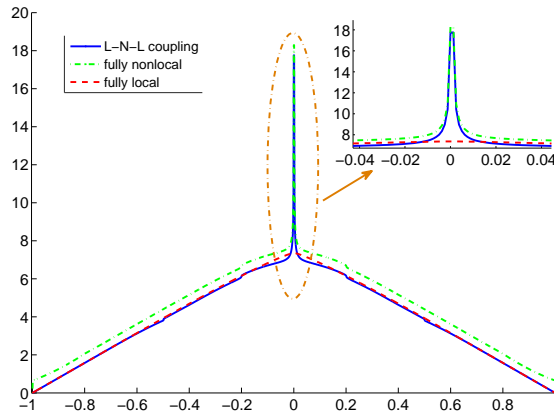


FIGURE 4. The solutions are plotted with mesh size $h = 1/800$, and horizon size $\delta = 0.2$. We fix the local-nonlocal-local coupling with interfaces at $x^a = -\frac{1}{2}$ and $x^b = \frac{1}{2}$. Kernel function is chosen to be $\gamma_\delta(x) = \frac{3}{2\delta^3}\chi_{(-\delta,\delta)}(x)$

6. CONCLUSION

By extending the idea of “geometric reconstruction” proposed in [15, 23], we developed a top-down quasinonlocal coupling method to study the nonlocal-to-local (NtL) diffusion problem in one

dimensional space. This new coupling framework removes interfacial inconsistency and maintains all physical properties at local continuum PDE levels, whereas none of existing coupling methods for nonlocal-to-local problems satisfies all of these properties. We proved the well-posedness of the coupling problem by a quasinonlocal version of the Poincaré inequality and established rigorous estimate of the modeling error by the maximum principle. Furthermore, we proposed a first order finite difference numerical discretization and confirmed the analysis by several numerical tests. The coupling formulation also removes artificial boundary effects caused by the fully nonlocal model when only classical Dirichlet boundary conditions are imposed. Although our discussions here have focused on scalar one dimensional model problems, it is natural to investigate whether similar ideas can be developed for systems of equations and for problems defined in multi-dimensions. Such generalizations are indeed possible and they will be carried out in separate works.

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